

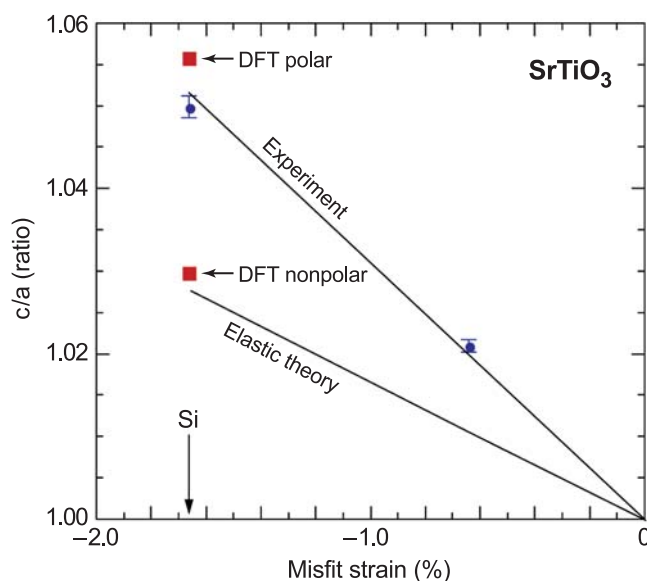
## Spectroscopy, Diffraction, and Imaging of Electronic Materials

*We are working to develop, establish, and provide synchrotron-based metrology, including instrumentation and technical expertise, for spectroscopy, diffraction, and imaging techniques applicable to the study of nanoscale and other phenomena that are important in the design, application, and performance of electronic materials.*

**Joseph C. Woicik**

The epitaxial growth of oxides on silicon opened the possibility of incorporating many of their unique electronic properties into silicon device technology. We have studied the epitaxy and lattice expansion of  $\text{SrTiO}_3$  thin films grown coherently on  $\text{Si}(001)$  by kinetically controlled sequential deposition. Coherent growth is achieved by repetition of the deposition sequence that includes a low-temperature and high-oxygen partial-pressure step followed by a high-temperature and low-oxygen partial-pressure step, thereby suppressing the detrimental oxidation of the silicon substrate.

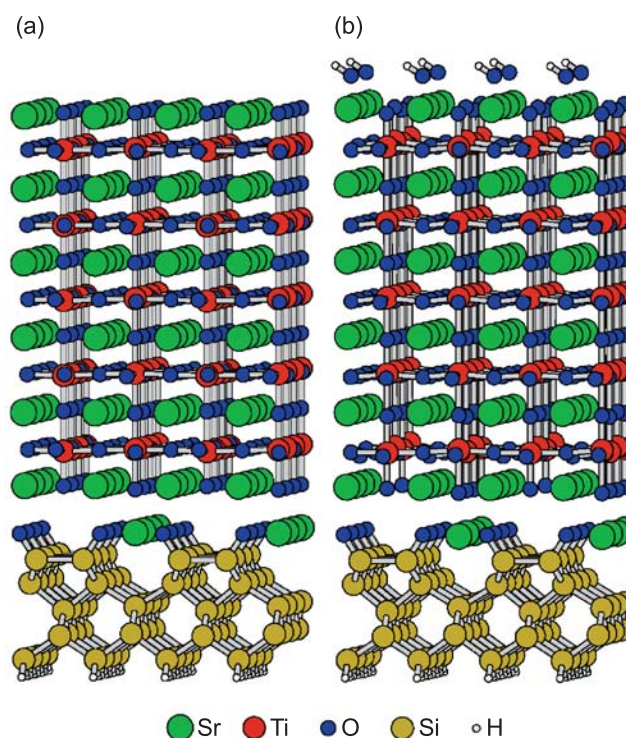
Unlike films grown by more traditional molecular-beam-epitaxy (MBE) methods, these films are found to have an in-plane lattice constant that is indistinguishable from the silicon substrate, an out-of-plane lattice constant that is expanded by an amount twice that predicted by the bulk elastic



**Figure 1:** Measured  $c/a$  ratio for 5 ML and 10 ML films as a function of in-plane lattice mismatch. Also shown are the predictions of elastic theory and density functional theory (DFT).

constants of  $\text{SrTiO}_3$ , and a critical-thickness behavior beyond  $\sim 2$  nm (5 unit cells or 5 monolayers (ML's)).

The experimentally determined  $c/a$ -ratio as a function of in-plane misfit strain is shown in Figure 1, for both 5 ML and 10 ML films. The experimental results are compared to the results of density functional theory for the  $c/a$  ratio of a 5 ML film in coherent registry with the silicon substrate as shown in Figure 2. The difference between the two structures in Figure 2 is the presence of OH adsorbates on the surface and oxygen vacancies at the interface, as revealed by high-resolution x-ray photoelectron spectroscopy for films that have been exposed to air.



**Figure 2:** Structure of the ideal 5 ML  $\text{SrTiO}_3/\text{Si}(001)$  system (a) and the system with O vacancies and OH adsorbates (b). Note the ferroelectric polarization in (b) but not in (a).

This energetically favorable interfacial-defect/surface-charge structure compensates the ferroelectric depolarization field and allows the ferroelectric polarization in these ultra-thin films that is confirmed by Ti K-edge x-ray absorption fine-structure measurements.

### Contributors and Collaborators

H. Li (Motorola Labs); P. Zschack, E. Karapetrova (UNICAT); P. Ryan (Ames Lab); C.R. Ashman, C.S. Hellberg (NRL); A. Allen, D. Black, M. Green, I. Levin (Ceramics Division, NIST)